The few-body problem for trapped bosons with large scattering length

S. Jonsell, H. Heiselberg, and C. J. Pethick
NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark
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We calculate energy levels of two and three bosons trapped in a harmonic oscillator potential with oscillator length $a_{\rm osc}$. The atoms are assumed to interact through a short-range potential with a scattering length a, and the short-distance behavior of the three-body wave function is characterized by a parameter θ. For large positive $a/a_{\rm osc}$, the energies of states which, in the absence of the trap, correspond to three free atoms approach values independent of a and θ. For other states the θ dependence of the energy is strong, but the energy is independent of a for $|a/a_{\rm osc}| \gg 1$.

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By exploiting the properties of Feshbach resonances, it has become possible to tune atomic scattering lengths to essentially any value, either repulsive or attractive [1]. This has led to renewed interest in the properties of systems with large scattering length a, a problem which has also been studied extensively in the context of nuclear physics, because the scattering lengths for nucleon-nucleon interactions are large in magnitude compared with the spatial scale r_0 of the interparticle interaction.

A novel possibility for exploring experimentally the properties of few-body systems is to trap atoms in a periodic potential created by standing-wave light beams, a so-called optical lattice. For example, in the experiments described in Ref. [2], up to $200,000$ ^{87}Rb atoms were distributed over more than $150,000$ lattice sites, thereby creating a large number of few-body systems with up to 2.5 atoms each on average. This provides one motivation for theoretical studies of few-body problems in traps. A second motivation is to understand theoretically the properties of bulk matter when the magnitude of the scattering length is large compared with the interparticle spacing $n^{-1/3}$, where n is the particle density. In this regime, the usual low density approximations, which are valid only if $n|a|^3 \ll 1$, fail. Recently, one has sought a universal description, with $n|a|^3$ as the only parameter, of the many-body problem for Fermi [3] and Bose [4] systems interacting via short-range potentials ($r_0 \ll n^{-1/3}$), but with $n|a|^3 \simeq 1$. Studies of three-body recombination in ultracold Bose gases have, however, revealed that the rate depends on an additional three-body parameter [5], and in a recent work, it has been suggested that the equation of state of a Bose gas in the limit $n^{-1/3} \ll |a|$ may depend on the three-body parameter [6]. Study of the few-body system in a trap is therefore of interest in order to obtain insights into the properties of bulk matter.

In this Letter we calculate the energy of systems with two or three identical bosons of mass m in a harmonic trapping potential $V_{\rm trap} = m\omega^2 r^2/2$, where ω is the frequency of oscillations of a particle about the minimum of the potential. The length associated with the zero-point motion of a particle in the trap is $a_{\rm osc} = \sqrt{\hbar/m\omega}$. The bosons are assumed to interact via a short-range potential. To take this into account, we impose the boundary condition $\partial \ln(r_{ij}\Psi)/\partial r_{ij}|_{r_{ij}\to 0} = -1/a$. Here $\Psi(\mathbf{r}_1, \ldots \mathbf{r}_N)$ is the wave function of the N-body system, $\mathbf{r}_i$ being the coordinates of the particles, and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$.

We first consider the two-body problem. Solving the Schrödinger equation for two bosons in a harmonic oscillator potential, one finds that the eigenenergies E, excluding the center of mass contribution, are given by [7]

$$\frac{a}{a_{\rm osc}} = \frac{1}{\sqrt{2}} \frac{\Gamma[1/4 - E/(2\hbar\omega)]}{\Gamma[3/4 - E/(2\hbar\omega)]}. \qquad (1)$$

For $a = 0$ the s-wave states have energies $E = \hbar\omega(2\nu + 3/2)$, $(\nu = 0, 1, \ldots)$ at which the gamma function in the denominator diverges, while for $a/a_{\rm osc} \to \pm\infty$, the energies are $E = \hbar\omega(2\nu + 1/2)$. Hence, when the bosons are confined to a volume smaller than $|a|^3$, the scattering length becomes unimportant. Interestingly, the energy does not increase without limit as a becomes large, as one would predict from the standard low-density result for the energy.

We now investigate the analogous problem for three trapped bosons, and adopt the method of Ref. [8]. The wave function of three identical bosons may be decomposed in the usual Faddeev fashion as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \psi(\mathbf{x}, \mathbf{y}) + \psi(\mathbf{x}', \mathbf{y}') + \psi(\mathbf{x}'', \mathbf{y}''). \qquad (2)$$

Here the Jacobi coordinates $\mathbf{x} = \mathbf{r}_{12}$, and $\mathbf{y} = \mathbf{r}_3 - (\mathbf{r}_1 + \mathbf{r}_2)/2$ have been used. If interactions between atoms are purely s-wave, ψ is a function of the hyperradius $\rho = (x^2/2 + 2y^2/3)^{1/2}$ and the hyperangle $\alpha = \arctan(\sqrt{3}x/2y)$ only. Variables related to the original ones by cyclic permutations of the particles are denoted by primes and double primes.

The wave function ψ may be represented exactly by an infinite sum

$$\psi(\rho, \alpha) = \frac{1}{\sqrt{3}} \sum_i \frac{f_i(\rho)}{\rho^{5/2}} \frac{\phi_i(\rho, \alpha)}{\sin\alpha\cos\alpha}, \qquad (3)$$

where $\phi_i(\rho, \alpha)$ are eigensolutions to the hyperangular part of the problem, which for a short-range potential reduce to

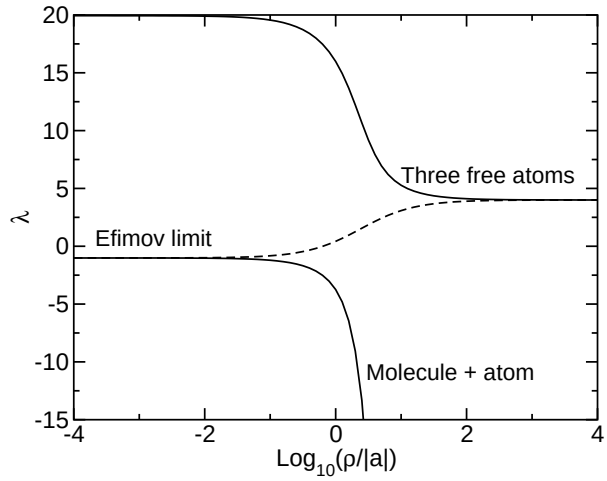

FIG. 1. Eigenvalue $\lambda_i(\rho/|a|)$ of the hyperangular equation for $a > 0$ (solid) and $a < 0$ (dashed).

$$\phi_i(\rho,\alpha) = \sqrt{N(\rho)}\sin\left[\sqrt{\lambda_i}(\alpha-\pi/2)\right]. \qquad (4)$$

The eigenvalues λ_i are determined by the boundary condition as $\alpha \to 0$, i.e. when two of the bosons approach each other, and are given by the equation

$$\sqrt{\lambda_i}\cos\left[\sqrt{\lambda_i}\frac{\pi}{2}\right] - \frac{8}{\sqrt{3}}\sin\left[\sqrt{\lambda_i}\frac{\pi}{6}\right] = \sqrt{2}\frac{\rho}{a}\sin\left[\sqrt{\lambda_i}\frac{\pi}{2}\right]. \qquad (5)$$

The hyperradial wave functions f_i are the solutions of an infinite number of coupled differential equations

$$\left(-\frac{\partial^2}{\partial\rho^2} + \frac{\lambda_i(\rho/a)-1/4}{\rho^2} - Q_{ii}(\rho) + \frac{\rho^2}{a_{\rm osc}^4} - \frac{2mE}{\hbar^2}\right) f_i(\rho) = \sum_{j\neq i}\left(Q_{ij}(\rho) + 2P_{ij}(\rho)\frac{\partial}{\partial\rho}\right) f_j(\rho). \qquad (6)$$

The effective potential for the hyperangular motion therefore depends on the eigenvalue λ_i associated with the hyperangular degrees of freedom. The coupling matrices are given by the kinetic-energy operator acting on the hyperangular wave functions:

$$P_{ij}(\rho) = \left\langle \Phi_i \left| \frac{\partial}{\partial\rho} \right| \Phi_j \right\rangle,\ Q_{ij}(\rho) = \left\langle \Phi_i \left| \frac{\partial^2}{\partial\rho^2} \right| \Phi_j \right\rangle, \qquad (7)$$

where $\Phi_i(\rho,\alpha,\alpha',\alpha'') = \phi_i(\rho,\alpha) + \phi_i(\rho,\alpha') + \phi_i(\rho,\alpha'')$. An approximation which has worked well in a number of applications [9] is to neglect the coupling terms P and Q. This is an adiabatic approximation in the sense that the hyperangular functions $\Phi_i(\rho,\alpha,\alpha',\alpha'')$ are assumed to vary much more slowly with hyperradius than with the hyperangles. The method can be refined by including coupling between a finite subset of states.

In Fig. 1 we plot $\lambda_i(\rho/|a|)$ calculated from Eq. (5) for some adiabatic states. For both $a > 0$ and $a < 0$ we show the state approaching $\lambda_i = 4$ for large $\rho/|a|$. This would, in the absence of the trap, correspond at large ρ to three free atoms, and it is the state of greatest interest in the present work. Also shown for $a > 0$ is the result for the state which would correspond to a diatomic molecule and an atom.

Let us now examine the form of the adiabatic hyperspherical wave functions. The functions of interest are ones which remain finite as $\rho \to 0$. The effective potential for small $\rho/|a|$ varies as $(\lambda_i(0) - 1/4)\rho^{-2}$. Consequently for $\lambda_i(0) > 0$ the hyperradial wave function f_i tends to zero as $\rho^{\sqrt{\lambda_i(0)}+1/2}$ for small $\rho/|a|$, and it does not depend on the nature of three-body correlations when no two atoms are separated by more than the typical range of the interaction. The situation is quite different for $\lambda_i(0) < 0$, since the effective potential is then attractive at small ρ. The two linearly independent solutions oscillate rapidly as $\rho \to 0$, but do not diverge, and the general solution for small ρ may be written

$$f(\rho) \to \sqrt{\rho}\sin[|s_0|\ln(\rho/a_{\rm osc}) + \theta], \qquad (8)$$

where $s_0 = \sqrt{\lambda_0(0)} \simeq 1.00624i$ and θ is a three-body parameter analogous to the phase shift for the two-body problem.

We turn now to the energy eigenvalues. In Fig. 2 we exhibit numerical results for the solution of Eq. (6), where the only states included are those shown in Fig. 1. For $a > 0$, coupling between the two hyperangular functions has been included. Since this is weak, it is still possible to separate states that for large ρ correspond to three free atoms from states that correspond to a molecule and an atom. We show the energy only of the states that for large ρ correspond to three free atoms, since these are the states of interest here.

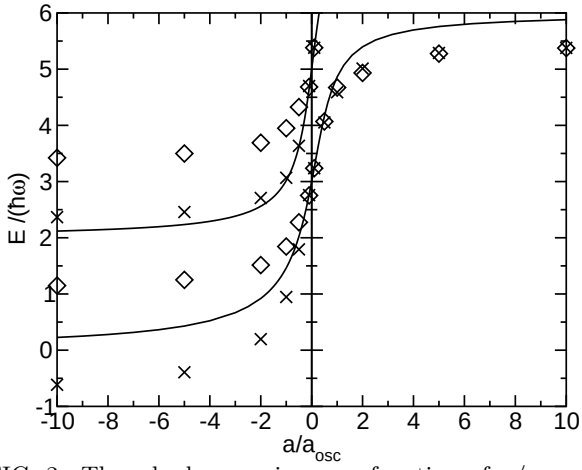

FIG. 2. Three-body energies as a function of $a/a_{\rm osc}$, for $\theta(\mathrm{mod}\,\pi) = 0$ (crosses) and $\theta(\mathrm{mod}\,\pi) = \pi/2$ (diamonds). For comparison the solid line shows the energy obtained when three-body correlations are neglected.

For small $|a/a_{\rm osc}|$ the energy of the lowest harmonic oscillator state can be expanded as

$$E = \hbar\omega \left[3 + \frac{6}{\sqrt{2\pi}} \frac{a}{a_{\rm osc}} + c \left(\frac{a}{a_{\rm osc}} \right)^2 + \dots \right]. \quad (9)$$

A lower bound to the energy may be found by omitting $Q_{ii}(\rho)$ in Eq. (6). An upper bound may be obtained by evaluating the energy for the trial wave function $f_i^{(0)}\Phi_i$, where $f_i^{(0)}$ is the solution of Eq. (6) in the absence of the coupling terms [10]. Including the same states as before, we find $-0.55 < c < -0.25$. For comparison, if three-body correlations are neglected, the correlation energy (the difference between the total energy and that of the corresponding state in the absence of interactions) is three times the correlation energy for two bodies, as obtained from Eq. (1). The resulting approximation for the energy has the same term linear in $a/a_{\rm osc}$, but the quadratic term has a different coefficient, $c = 6(1 - \ln 2)/\pi \simeq 0.59$. Hence, three-body effects are to leading order proportional to $(a/a_{\rm osc})^2$.

With increasing $|a|/a_{\rm osc}$ the dependence of the energy on θ grows. For $a < 0$ this is due to the sensitivity of the adiabatic state to the inner boundary condition. The adiabatic state for $a > 0$ is insensitive to θ, and the θ dependence arises due to coupling to states having different hyperangular functions. Energies for $\theta = 0$ and $\theta = \pi/2$ are compared in Fig. 2, and the difference grows with $a/a_{\rm osc}$ until $a/a_{\rm osc} \sim 1$, where it is $\sim 5\%$ of the correlation energy. At larger values of $a/a_{\rm osc}$ the θ dependence decreases. This is an effect of the confining potential. The hyperradial wave function $f(\rho)$ varies on a scale $\sim a_{\rm osc}$. As shown above, the hyperangular wave function Φ_i does, however, depend on the hyperradius through the combination ρ/a. Hence the couplings P and Q Eq. (7) are suppressed by factors $a_{\rm osc}/a$ and $(a_{\rm osc}/a)^2$ respectively when $a > a_{\rm osc}$.

The θ dependence of the energy is shown in more detail in Fig. 3 for $a > 0$. Physical conditions only determine $\theta (\mathrm{mod}\, \pi)$, but to exhibit the structure we have continued the energy curves over a larger range of θ. Hence, given values of $a/a_{\rm osc}$ and θ, $E(\theta)$, $E(\theta+\pi)$, $E(\theta+2\pi)$ etc. along the same curve represent the energies of different physical states. States corresponding mainly to free atoms at large ρ are represented by the nearly θ-independent segments of the curves. In the adiabatic approximation, i.e. neglecting all couplings, these states have energies shown by the dotted lines. Energies of other states, i.e. states associated with molecular bonding, are given by the dashed lines. The difference between the solid and dashed/dotted lines is the effect of the couplings between the two hyperangular functions. The couplings are most important when $a \simeq a_{\rm osc}$, and are almost entirely absent for $0 < a < 0.1a_{\rm osc}$ and $a > 10a_{\rm osc}$. The results for $a = 10a_{\rm osc}$ indicate that for $a \gg a_{\rm osc}$ the couplings vanish and our solution becomes exact.

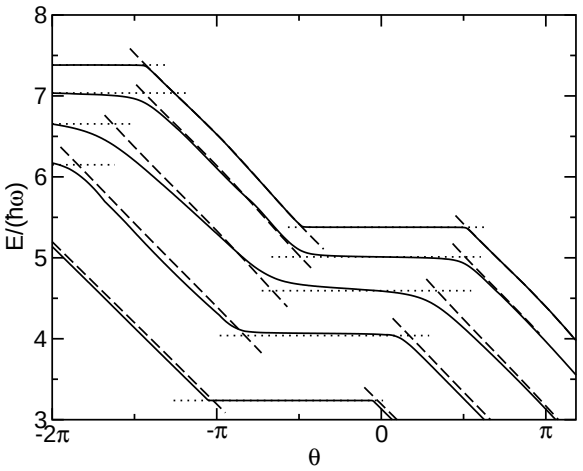

FIG. 3. Energy of θ for (from below) $a/a_{\rm osc} = 0.1$, 0.5, 1, 2, and 10. Dashed and dotted lines show energies in the adiabatic approximation, i.e. neglecting couplings between hyperangular functions. θ has been extended over several branches π in order to simultaneously show several physical states (see text).

In the limit $a/a_{\rm osc} \to \pm\infty$ Eq. (6) may be solved exactly. The energy tends to a constant value, which for the lowest state with a given $\lambda_i(0) > 0$ is $E = \hbar\omega(1 + \sqrt{\lambda_i(0)})$. For the state which at large ρ corresponds to free atoms, and for $a > 0$, one has $\lambda_i(0) \simeq 19.94$ and $E \simeq 5.47\hbar\omega$. The corresponding energy if only two-body correlations are included is $E = 6\hbar\omega$, and therefore the correlation energy is reduced by approximately 18% by three-body effects. For $\lambda_i(0) < 0$ the energies are functions of the boundary condition for $\rho \to 0$, i.e. of θ, and are given by the solutions of the equation

$$\theta = -\arg \left\{ \frac{\Gamma[1/2 - E/(2\hbar\omega) - s_0/2]}{\Gamma[1 - s_0]} \right\}. \quad (10)$$

For $E > 0$ this equation gives harmonic oscillator states shifted by the interaction, with spacings $E_{n+1} - E_n \simeq 2\hbar\omega$, while for $E < 0$ it gives bound three-body states, so-called Efimov states with energies scaling like $E_{n+1}/E_n = \exp(2\pi/|s_0|) \simeq 515$ [11] perturbed by the oscillator potential. For example $\theta = 0$ gives energies $E \simeq \dots$, $-291649\hbar\omega$, $-566\hbar\omega$, $-0.85\hbar\omega$, $2.27\hbar\omega$, $4.48\hbar\omega$, $\dots$.

Let us now examine the implications of our results for the properties of bulk matter. On physical grounds, we would expect the energy per particle in trapped few-body systems to be similar to that for bulk matter if the oscillator length is replaced by the typical particle separation. For $|a| \gg a_{\rm osc}$, the energy per particle of two- and three-body states for which $\lambda_i(0) > 0$ is $\sim \hbar\omega$ greater than in the absence of interactions. Since the density of particles is $n \sim 1/a_{\rm osc}^3$, this corresponds to an energy per particle $\sim (\hbar^2/m)n^{2/3}$. There is no dependence on θ for these states. The state corresponding to unbound atoms in a trap falls into this class for positive a. This suggests that

the energy per particle of bulk matter has the universal dependence $\sim Cn^{2/3}$, where C is a constant that does not depend on the three-body parameter θ. In particular, it does not have density-dependent contributions that are periodic in $\ln n$, contrary to the possibility suggested in Ref. [6]. There are other states, such as those associated with molecular states bound by the interatomic potential, which do exhibit a strong dependence on θ. These latter states are the final states in recombination processes, where diatomic molecules are formed from free atoms, and consequently recombination rates depend strongly on θ.

The expansion Eq. (9) of the energy of three trapped bosons, may be compared to the low-density expansion for the energy of N bosons in a homogenous gas [12]

$$E = \frac{2\pi\hbar^2 an}{m}(N-1)\left[1 + \frac{128}{15}\left(\frac{na^3}{\pi}\right)^{1/2} + \dots\right]. \quad (11)$$

For comparison, our result Eq. (9) for the energy of three trapped bosons with $|a/a_{\rm osc}| \ll 1$, may be rewritten as

$$E = 3\hbar\omega + \frac{2\pi\hbar^2 a\bar{n}}{m}(N-1)\left[1 + \frac{c\sqrt{2\pi}}{6}\frac{a}{a_{\rm osc}} + \dots\right]. \quad (12)$$

Here the average density, weighted by the particle number, is defined by $\bar{n} = \int n(\mathbf{r})dN(\mathbf{r})/\int dN(\mathbf{r}) = \int n^2(\mathbf{r})d\mathbf{r}/N$, where $dN(\mathbf{r}) = n(\mathbf{r})d\mathbf{r}$, and therefore for a homogeneous condensate $\bar{n} = n$. The three-body and many-body results agree for the term linear in a, which usually is the only term retained in, e.g. the Gross-Pitaevskii equation for condensates. Beyond the linear term the two expansions differ. The next term in Eq. (11) is of order $(na^3)^{1/2}$ relative to the first one, while in Eq. (12) it is proportional to $a/a_{\rm osc}$. If $N \lesssim a_{\rm osc}/a$ the most important correction to the linear dependence of energy on a will be the second term in Eq. (12), which arises from the trapping potential.

To determine when the three-body parameter θ becomes important, we note that, in the absence of the trap, the S-matrix element between the adiabatic state corresponding to free atoms and that corresponding to a diatomic molecule and an atom is proportional to $(ka)^2$, where k is the wave number of the colliding atoms. Therefore the recombination rate is proportional to a^4, in agreement with earlier work [5]. The constant of proportionality depends on θ, because of the θ dependence of the final state. The same result is valid in a trap with $a_{\rm osc} \gg |a|$, where due to the zero point motion k is of order $1/a_{\rm osc}$. Therefore, the first term in the small $a/a_{\rm osc}$ expansion of the energy [Eq. (9)] that depends explicitly on the coupling between different adiabatic states (and therefore on θ) is of order $(a/a_{\rm osc})^4$. In the expansion Eq. (12) this corresponds to the cubic term, since there one power of $a/a_{\rm osc}$ has been factored out. To this order the result agrees with the results for the energy density of the homogeneous Bose gas in Ref. [13]. As we saw above, for $a \gg a_{\rm osc}$ the couplings P and Q between hyperangular functions are *reduced*, which will tend to suppress recombination rates.

In conclusion, we have found that there are states of the trapped three-boson system with very weak dependence of the energies on the three-body parameter θ. This dependence vanishes completely in the limit of an infinitely large scattering length. The fact that the energy of these states is independent of the three-body parameter in the limit of large scattering lengths gives some grounds to hope that the energy of trapped systems with a larger number of bodies is insensitive to the parameters describing the four- and higher-body problems, and that similar conclusions apply to the energy of bulk matter. Topics for future study include higher-body correlations, and the lifetime of a condensate with a large scattering length.

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